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ANALYTIC CROSS SECTIONS FOR

$1^1S \rightarrow 1^1S$, $1^1S \rightarrow 2^1S$, $1^1S \rightarrow 2^1P$

TRANSITIONS IN HELIUM BY ELECTRON IMPACT

(NASA-CR-131265) ANALYTIC CROSS SECTIONS FOR 1 1S, TO 1 1S TO 2 1S, 1 1S TO 2 1P TRANSITIONS IN HELIUM BY ELECTRON IMPACT (Pittsburgh Univ.) 18 p HC $3.00 CSCL 20H G3/24
N73-20761
Unclas
17248

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ABSTRACT

The $1^1S \rightarrow 1^1S$ elastic and $1^1S \rightarrow 2^1S$ and $1^1S \rightarrow 2^1P$ excitation cross sections of Helium atoms by collision with a charged particle are obtained as analytic functions of incident velocity. The first order time dependent scattering theory is used. Numerical values of e^--He cross sections are obtained for incident energies in the range (30 eV - 800 eV) and compared with earlier Born approximation calculations and with available experimental data. It is found that at 100 eV and above, the present results are in good agreement with the experimental results of Vriens et al (1968) for elastic scattering, of Lassattre (1965) for $1^1S \rightarrow 2^1S$ and of Vriens et al (1968) for $1^1S \rightarrow 2^1P$ excitations. They are also closer to the experimental results than the corresponding Born calculations.

1. Introduction

In this paper we use the first order time dependent scattering theory to evaluate optically allowed and forbidden transition cross sections in atomic He by collision with a charged particle. This method was first used in atomic collision problems by Seaton[1] (1963) who pointed out the superiority of the cross sections thus obtained over that given by the usual Born approximation. Subsequently other authors have used the method to calculate cross sections for many optically allowed transitions[2] and for transitions mediated by the quadrupole force[3].

These early works are characterized by two further approximations within the framework of a first order theory. First, the exact Coulomb interaction is replaced by an outer expansion in terms of multipole moments and second, a cut off parameter is introduced on plausible physical grounds to prevent the cross sections from growing indefinitely at small impact parameters. These two approximations are related in the sense that the multipole potential, valid for relatively larger distances, necessarily diverges when extended down to the origin. It is this divergence which the cut off parameter is designed to prevent. The use of multipole expansion also limits the kind of cross sections that can be calculated by this method. For example, the optically forbidden $1S \rightarrow 2S$ transitions in H or $1^1S \rightarrow 2^1S$ in He cannot be evaluated from such a potential (due to the vanishing of the relevant matrix elements). Recently the semiclassical method has been extended to calculations of such and other cross sections by the more elaborate and in principle more accurate method of solving the (time dependent) close coupling equations[4]. As is well known, unlike the first order theory, this involves extensive numerical computations. We therefore, consider it worthwhile to investigate the use of the first order theory in predicting analytically optically forbidden as well as allowed transitions in He. Reexamining the first order theory in the line indicated above we find that if no approximation is made of the interaction potential, then the unsatisfactory divergences (and the associated problem of choosing a (non-unique) cut off parameter) can be eliminated. At the same time, the cross sections for all transitions, including the optically forbidden ones, can still be obtained directly as analytic functions of the incident energy. In this work, to illustrate the procedure we have evaluated the elastic $1^1S \rightarrow 1^1S$ and the inelastic $1^1S \rightarrow 2^1S$ and $1^1S \rightarrow 2^1P$ cross sections in He (for electron impact) and compared them with the available experimental results and with calculations under Born approximation.

2. Theory

The transition probability in the first order time dependent perturbation theory is given by

$$P_{i\to J} = \frac{1}{\hbar^2 S_i} \sum \left| \int_{-\infty}^{\infty} e^{iwt} \; V_{i\to J}(t)dt \right|^2 \tag{1}$$

where

$$V_{i\to J}(t) = \int d\vec{r}_p \; \phi_J^*(\vec{r}_p) \left\{ \frac{Z\,Z_o e^2}{r(t)} - \sum_{p=1}^{Z} \frac{Z_o e^2}{|\vec{r}(t)-\vec{r}_p|} \right\} \phi_i(\vec{r}_p)$$

ϕ_i and ϕ_J are initial and final wavefunctions, S_i is the statistical weight of the state i and the summation is over the degenerate initial and final states of the target; $\hbar w = E_i - E_f$, Z_o is the charge on the incident particle and Z is the nuclear charge of the atom. The motion of the incident particle is described by the classical trajectory $\vec{r}(t)$ which we assume to be a straight line along the z-axis.

$$r^2(t) = b^2 + (vt)^2 \tag{3}$$

where b is the impact parameter v is the velocity and t stands for time.

We have adopted the following analytic Hartree-Fock wave functions for the He atom[4,5].

$$\psi_{1^1S}(\vec{r}_1, \vec{r}_2) = \frac{N_{1S}}{\pi} \; \phi_{1S}(r_1)\phi_{1S}(r_2) \tag{4}$$

where

$$\phi_{1S}(r) = \exp(-\alpha r) + B \exp(-Br) \tag{5}$$

with

$N_1 = 1.6966$ $\qquad$ $B = 0.7990$

$\alpha = 1.41$ $\qquad$ $\beta = 2.61$

$$\psi_{2^1S}(\vec{r}_1,\vec{r}_2) = \frac{N_{2S}}{\pi} \{\exp(-2r_1)\, \phi_{2S}(r_2) + \exp(-2r_2)\, \phi_{2S}(r_1)\} \tag{6}$$

where

$$\phi_{2S}(r) = \exp(-\gamma r) + Dr \exp(-\delta r) \tag{7}$$

with $N_{2S} = 0.70638$ $\qquad$ $D = -0.26832$

$\gamma = 1.1946$ $\qquad$ $\delta = 0.4733$

which is orthogonal to the ground state wave function (4).

$$\psi_{2^1P_m}(\vec{r}_1,\vec{r}_2) = \frac{N_{2p}}{\pi^{1/2}} \{\exp(-2r_1)\, \phi_{2p_m}(\vec{r}_2) + \exp(-2r_2)\, \phi_{2p_m}(\vec{r}_1)\} \tag{8}$$

where

$$\phi_{2p_m}(\vec{r}) = r \exp(-\lambda r)\, Y_{1m}(\hat{r}) \tag{9}$$

with

$$N_{2p} = 0.37831 \qquad \lambda = 0.485,$$

and $Y_{1m}(\hat{r})$ is a spherical harmonic .

For the eigen energies we have adopted the experimental values[5]

$$E_{1^1S} = 2.90372 \qquad E_{2^1S} = 2.14597$$

$$E_{2^1P} = 2.12384.$$

First, using the above wave functions the transition potentials (2) are calculated. Substituting these (time dependent) potentials in (1) the integration over time is performed analytically to obtain the expressions for the transition probabilities which are given in the appendix. The respective cross sections are then obtained from the expression[6]

$$\sigma_{if}(E) = \frac{V_f}{V_i} \int_0^\infty P_{iJ}(b)\, 2\pi b\, db \tag{10}$$

It is to be noted that the above definition of transtion cross sections automatically satisfies the quantum - mechanical reciprocity relation, provided the velocity of the projectile in its entire trajectory is taken to be an average of the velocities before and after the collision, which we set simply equal to the mean velocity

$$V = \frac{V_i + V_f}{2} \tag{11}$$

This choice further fulfills the requirement that the transition cross sections (10) vanish at the thresholds.

We now carry out the integrations over the impact parameters in (10) and obtain the $\sigma_{1^1s \to 1^1s}$, $\sigma_{1^1s \to 2^1s}$ and $\sigma_{1^1s \to 2^1p}$ cross sections in terms of the well known Gauss - hypergeometric functions. The method of obtaining the final results are described in the appendix and the full expressions are obtainable from the authors on request. Inspite of their lengths the expressions are basically simple.

3. Discussion:

In Tables 1, 2 and 3 we give representative values for the elastic $1^1s \to 1^1s$ cross sections and the inelastic $1^1s \to 2^1s$ and $1^1s \to 2^1p$ cross sections in He by e^- impact. To compare we also quote results of previous Born calculations[5] using the same wave functions and several experimental measurements[7-11].

Table 1. Cross sections for the elastic scattering of electrons by He (in πa_0^2)

Energy (ev)	Present Results	Experiment[a]	First Born[b]	Simplified Second Born (complete)[b]
50	0.9598			
100	0.4799	0.76	0.411	0.893
150	0.3199	0.44	0.288	0.514
200	0.2399	0.31	0.222	0.352
300	0.1600	0.19	0.152	0.211
400	0.1200	0.142	0.1154	0.1489
500	0.0960		0.0931	0.1146

[a]Vriens et.al. (ref. 7)

[b]Holt et. al. (Ref. 5)

Table 2. Cross Sections for the

Excitation 1's → 2's of He by electrons.

(in $10^{-3}\,\pi a_o^2$)

Energy in ev	Present Results	Expt[a]	Expt[b]	First[c] Born	Simplified[c] Second Born (complete)
30	44.22				
50	36.24				
80	25.30				
100	20.88	21.0		21.8	22.8
150	14.46	15.0		15.1	15.4
200	11.04	11.2	7.7	11.49	11.63
300	7.49	7.6	6.0	7.79	7.84
400	5.66	5.7	4.8	5.89	5.92
500	4.55			4.74	4.75
700	3.27			3.41	3.42

[a] Lassettre (Ref. 9)

[b] Vriens et.al. (Ref. 8)

[c] Holt et.al. (Ref. 5)

Table 3. Cross Sections for the Excitation 1's → 2'p of He by Electrons (in $10^{-2}\ \pi a_o^2$)

Energy ev	Present Results	Expt[a]	Expt[b]	First Born[c]	Simplified Second Born[c]
50	16.97		9.95		
80	16.09		11.70		
100	14.96	14.0	11.60	15.09	15.91
150	12.52	11.9	10.46	12.63	12.64
200	10.75	10.4	9.30	10.85	10.67
300	8.45	8.2	7.40	8.55	8.34
400	7.02	6.9	6.29	7.12	6.94
600	5.32	5.2	4.86	5.37	5.25
800	4.33	4.3	4.02	4.38	4.29

[a] Vriens Et.Al. (Ref. 8)

[b] Donaldson Et. Al. (Ref. 11)

[c] Holt Et.Al. (Ref. 5)

It would be seen from the tables that the results for all the three cross sections are in good agreement with experimental measurements above 100 e.v. They are at the same time closer to the experimental results than the quantal Born calculations. At energies below 100 e.v the disagreement with experiment (in the available case of 1's $\rightarrow$ 2'p transition) is marked. This disagreement at lower energies is perhaps to be expected, for the first-order perturbations theory is unlikely to be valid at such energies. Both the influence of exchange processes and the polarisation of the target atom, which are neglected in the present calculations, are likely to be important at such energies and the use of the second order perturbation theory alone is unlikely to be sufficient (Notice e.g. the difference between the second Born results and the experimental values even at 100 e.v)

We expect, however, that at 100 ev. and above the present analytic results would be useful for rapid and reliable calculations of similar cross sections given here. Finally we note that the above results apply directly for collisions with charged particles other than electrons (e.g. e^{+} and H^{+}) when the appropriate centre of mass velocities are used for the projectile.

APPENDIX

$$V_{1^1s\to 2^1s}(R) = \int \psi^{x}_{2^1s}(\vec{r}_1,\vec{r}_2)\left[\frac{2}{R} - \frac{1}{|\vec{R}-\vec{r}_1|} - \frac{1}{|\vec{R}-\vec{r}_2|}\right]\Psi_{1^1s}(\vec{r}_1,\vec{r}_2)$$

where $\vec{R}(t)$ is the position vector of the incident e^- referred to the Helium nucleus.

$$V_{1^1s\to 2^1s}(R) = 32\, N_{1s}\, N_{2s}\, [I_1(\alpha+2,\ \alpha+\gamma) + D\, I_2(\alpha+2,\ \alpha+\delta)$$

$$+ B^2\{I_1(\beta+2,\ \beta+\gamma) + D\, I_2(\beta+\gamma,\ \beta+\delta)\}$$

$$+ B\{I_1(\alpha+2,\ \beta+\gamma) + I_1(\beta+2,\ \alpha+\gamma)\}$$

$$+ BD\{I_2(\alpha+2,\ \beta+\delta) + I_2(\beta+2,\ \alpha+\delta)\}]$$

where

$$I_1(p,q) = \frac{2}{p^2q^2}\left[\frac{\exp(-pR)}{q}\left(1+\frac{2}{pR}\right) + \frac{\exp(-qR)}{p}\left(1+\frac{2}{qR}\right)\right]$$

$$I_2(p,q) = \frac{2}{p^2q^2}\left[\frac{3}{q^2}\exp(-pR)\left(1+\frac{2}{pR}\right)\right.$$

$$\left. + \frac{\exp(-qR)}{p}\left(R + \frac{4}{q} + \frac{6}{q^2R}\right)\right].$$

$$V_{1^1s\to 1^1s}(R) = 16N^2_{1s}\, [I_1(2\alpha,\ 2\alpha) + B^4\, I_1(2\beta,\ 2\beta)$$

$$+ 4B^2\, I_1(\alpha+\beta,\ \alpha+\beta) + 4B\, I_1(2\alpha,\ \alpha+\beta)$$

$$+ 4B^3\, I_1(2\beta,\ \alpha+\beta) + 2B^2\, I_1(2\alpha,\ 2\beta)]$$

$$V_{1^1s\to 2^1Pm}(R) = N_{2p}\, N_{2s}\, \frac{64}{3}(\pi)^{1/2}\ Y_{1m}(\theta,\phi)$$

$$[I_3(\alpha+2,\ \alpha+\lambda) + I_3(\beta+2,\ \beta+\lambda)$$

$$+ B\{I_3(\alpha+2,\ \beta+\lambda) + I_3(\beta+2,\ \alpha+\lambda)\}]$$

where

$$I_3(p,q) = \frac{3}{p^3q^2}\left[\frac{8}{q^3R^2} - \exp(-qR)\left\{\frac{8}{q^3R^2} + \frac{8}{q^2R} + \frac{4}{q} + R\right\}\right]$$

$$P_{1's\to 2's}(b) = 32N_{1s}N_{2s}\,[I_4(\alpha + 2; \alpha + \gamma) + DI_5\,(\alpha + 2, \alpha + \delta)$$

$$+ B^2\,\{I_4(\beta + 2, \beta + \gamma) + DI_5(\beta + \gamma, \beta + \delta)$$

$$+ B\,\{I_4(\alpha + 2, \beta + \gamma) + I_4(\beta + 2, \alpha + \gamma)$$

$$+ BD\,\{I_5(\alpha + 2, \beta + \delta) + I_5(\beta + 2, \beta + \delta)\}]$$

where b is the impact parameter defined in eq. 3 and

$$I_4(p,q) = \int_{-\infty}^{\infty} e^{iwt}\, I_1(p,q)\, dt$$

$$= \frac{4}{v}\frac{1}{p^2q^2}\left[\left\{\frac{p}{q}\frac{K_1(\beta_1 b)}{\beta_1} + \frac{q}{p}\frac{K_1(\beta_2 b)}{\beta_2}\right\}b\right.$$

$$\left. + \frac{2}{pq}\{K_o(\beta_1 b) + K_o(\beta_2 b)\}\right]$$

with

$$\beta_1 = \sqrt{p^2 + w^2/v^2}$$

$$\beta_2 = \sqrt{q^2 + w^2/v^2}$$

and

$$I_5(p,q) = \frac{4}{v}\left[\frac{1}{pq^2}\left\{\frac{3K_1(\beta_1 b)}{q^2\beta_1} + \frac{1}{p^2}\beta_3\frac{K_1(\beta_2 b)}{\beta_2}\right\}b\right.$$

$$+ \frac{6}{p^3q^4}\{K_o(\beta_1 b) + K_o(\beta_2 b)\}$$

$$\left. + \frac{K_o(\beta_2 b)}{p^3\beta_2{}^2}\, b^2\right]$$

with $\beta_3 = 4 + \frac{q^2 - w^2/v^2}{q^2 + w^2/v^2}$

$$P_{1s\to 1s}(b) = 16N_{1s}^2\,[I_4(2\alpha,2\alpha) + B^4\,I_4(2\beta,2\beta)$$

$$+ 4B^2\,I_4(\alpha+\beta,\,\alpha+\beta) + 4B\,I_4(2\alpha,\alpha+\beta)$$

$$+ 4B^2\,I_4(2\beta,\,\alpha+\beta) + 2B^2\,I_4(2\alpha,2\beta)]$$

$$P_{1s\,2Pm}(b) = N_{2p}N_{2s}\,(\pi)^{1/2}\,\frac{64}{3}\,[I_{6_m}(\alpha+2,\,\alpha+\lambda)$$

$$+ I_{6_m}(\beta+2,\,\beta+\lambda) + B\{I_{6_m}(\alpha+2,\,\beta+\lambda) + I_{6_m}(\beta+2,\,\alpha+\lambda)\}]$$

where

$$I_{6_o}(p,q) = \frac{2}{i}\,\frac{w}{v}\,\frac{1}{v}\;\frac{3}{4\pi}\,\frac{3}{p^3q^2}\,[\frac{8}{q^3}\{K_o(\beta_2 b) - K_o(\beta_4 b)\}$$

$$+ (\frac{4}{q}\,\frac{1}{\beta_2} + \frac{2q}{\beta_2^{\,3}})\,K_1(\beta_2 b)\,b$$

$$+ \frac{q}{\beta_2^{\,2}}\,K_o(\beta_2 b)\,b^2]$$

with $\beta_4 = w/v$.

$$I_{6_{\pm 1}}(p,q) = \mp\frac{2}{v}\;\frac{3}{8\pi}\;e^{i\phi}\,\frac{3}{p^3q^2}\,[\frac{8}{q^3}\{\beta_2K_1(\beta_2 b) - \beta_4K_1(\beta_4 b)\}$$

$$+ \frac{4}{q^2}\;Ko\,(\beta_2 b)\,b + \frac{K_1(\beta_2 b)}{\beta_2}\;b^2]$$

Finally, when these expressions for the transition probabilities are used in eq. (10) for the cross section, the integrals that arise are of the forms (a) and (b) where

(a)
$$\int_0^\infty b^{-\lambda} K_\mu(pb)\, K_v\,(qb)\, db$$

$$= 2^{-2-\lambda} \frac{p^{-v+\lambda-1}\, q^v}{\Gamma(1-\lambda)}\, \Gamma\left(\frac{1-\lambda+\mu+v}{2}\right) \Gamma\left(\frac{1-\lambda-\mu+v}{2}\right)$$

$$\Gamma\left(\frac{1-\lambda+\mu-v}{2}\right)\, \Gamma\left(\frac{1-\lambda-\mu-v}{2}\right)\, {}_2F_1\left(\frac{1-\lambda+\mu+v}{2}, \frac{1-\lambda-\mu+v}{2};\right.$$

$$\left. 1-\lambda;\, 1-\frac{q^2}{p^2}\right)$$

for $\operatorname{Re}\lambda < 1 - |\operatorname{Re}\mu| - |\operatorname{Re} v|$

where ${}_2F_1$ is the gauss hypergeometric function.

(b)
$$\int_0^\infty [\beta_1 K_1\,(\beta_1 b) - \beta_2 K_1\,(\beta_2 b)]\, \beta_3 K_1\,(\beta_3 b) b\, db$$

$$= \frac{\beta_3^{\,2}\ln\beta_3 - \beta_1^{\,2}\ln\beta_1}{\beta_1^{\,2} - \beta_3^{\,2}} - \frac{\beta_3^{\,2}\ln\beta_3 - \beta_2^{\,2}\ln\beta_2}{\beta_2^{\,2} - \beta_3^{\,2}} \quad \text{if } \beta_3 \neq \beta_1 \text{ or } \beta_2$$

$$= \frac{\beta_3^{\,2}\ln\beta_3 - \beta_1^{\,2}\ln\beta_1}{\beta_1^{\,2} - \beta_3^{\,2}} + \ln(\beta_2) + \frac{1}{2} \qquad \text{if } \beta_3 = \beta_2.$$

ACKNOWLEDGEMENTS

We would like to thank Prof. E. Gerjuoy for his clarifying comments on the semiclassical method. This work was supported by the National Aeronautics and Space Administration under contract No. NGR-39-011-150.

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